Usage Report for Fiscal Year 2024

Project Title:

Electron-phonon mediated superconductivity

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1. Background and purpose of the project, relationship of the project with other projects

This project explores electron-phonon interactions in superconductivity using many-body perturbation theory. In the community of superconductors, only the phonon-mediated superconductors bear sophisticated and accurate predictions from a first-principles calculation perspective. We aim to identify potential high-temperature superconductors, analyze phonon-electron coupling, and quantify the critical temperature (Tc) in selected novel materials.

2. Specific usage status of the system and calculation method

For the calculation of electronic structure and phonon band structure calculation, we require large memory and parallel computing to reduce the computational effort. The programs in specific that we have used are: Vienna Ab initio Package (VASP), Quantum Espresso (QE), Phonopy, and QE-Electron-Phonon-Wannier (EPW). We compute the electronic band structures calculation based on the density functional theory and the phonon, as well as electron-phonon coupling is calculated by the density functional perturbation theory.

3. Result

The material in particular we are interested in is the MgB_2 system. It is known to obtain a Tc of around 39K and can be well-explained by electron-phonon mechanism. Recently topological phonons are also very hop topic, and therefore we check whether there could be topological phonon enhanced surface superconductivity. If the phonon band is topological, we can have surface phonon modes. Thus, if there is a frequency gap that has isolated surface phonon bands, we could possibly quantify the surface phonon-mediated superconductivity in this region.

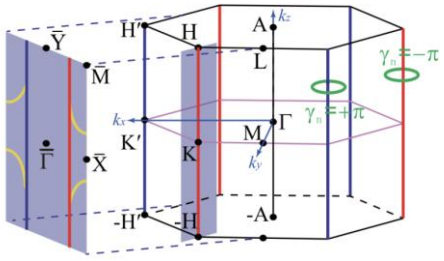

Figure 1. Bulk and surface brillouin zone of MgB_2 and slab model on [001] and [100].

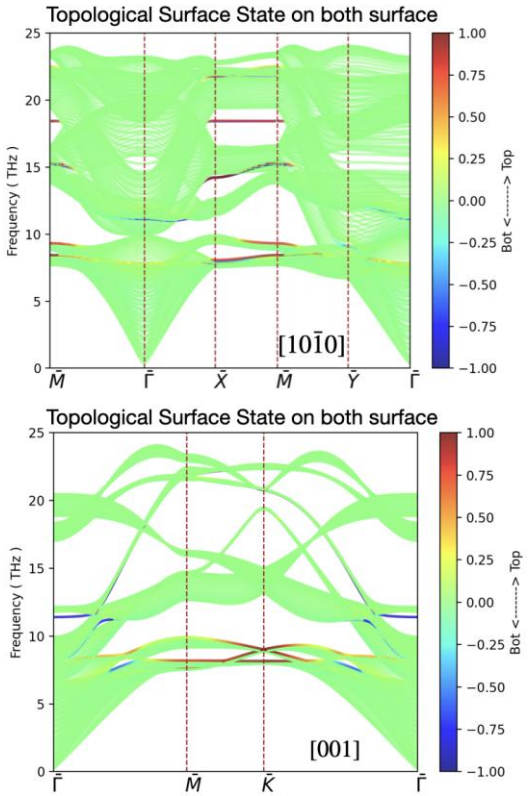

Figure 2. Topological phonon surface state for MgB_2 on [001] and [100].

Here, I will show the results of electron-phonon coupling of slab MgB_2 at the different facet, namely the [001] and [100] direction. The Brillouin zone definition is given in Figure 1. The behavior of surface state is shown in Figure 2. We could see that

the topological phonon surface states are more clearly seen, which is obvious in the bulk gap region around 15 and 20 THz for the [100] direction. Then what would the electron-phonon behavior be like? Below we show the electron-phonon calculation results for the bulk and 6 monolayer MgB_2. Although from literature, we know that the isotropic Eliashberg function is not suitable for the estimation of T_C; but here we use this as a first approach to estimate the electron-phonon coupling strength (λ).

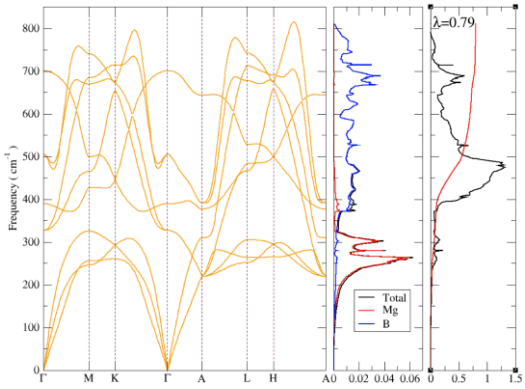

Figure 3: Phonon bands (left), phonon density of states (middle), and Eliashberg spectral function (right) for bulk MgB_2.

From the bulk MgB_2, as shown in Figure 3, we realize that the Eliashberg function is strongly contributed by the Boron ring in the region of 400~500 cm^{-1}. This is because the strong bonding of the Boron ring brings strong electron-phonon coupling, stabilizing the phonon-mediated superconducting gap. Next we look into the 6 monolayers MgB_2 cut at the [100] and [001] direction. The results are collected in Figure 4. Note that the [100] case supposedly have more distinct surface phonon mode as indicated from the surface phonon band.

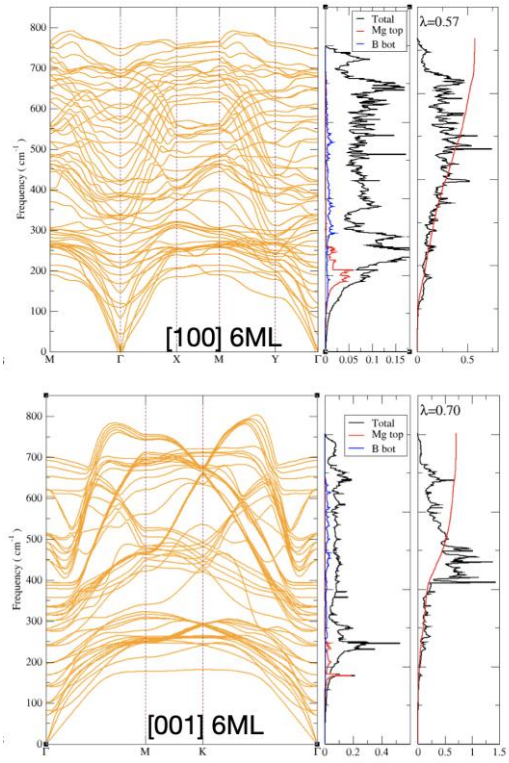

Figure 4: Phonon bands (left), phonon density of states (middle), and Eliashberg spectral function (right) for 6 monolayers MgB_2 along the [001] and [100] directions.

Surprisingly, the electron-phonon coupling of [001] direction is similar to that of bulk; on the other hand, the [100] direction is significantly lower with a difference of 0.2 in the λ. By comparing the peak of the Eliashberg function to the phonon density of states, we notice that the reason of this difference comes from mainly the Boron phonon. With these results, we can deduce that the significant topological phonon states observed in the [100] is due to the breaking of the Boron bond. This leads to dangling bonds and thus an obvious topological phonon states. However, what is important in the electron-phonon coupling of MgB_2 is the strong bonding coming from the hexagonal B network. Thus, the appearance of topological phonon state is presumably against the enhancement of possible surface superconductivity.

4. Conclusion

In this project, we investigated the possibility of

enhancing surface phonon-mediated superconductivity by topological phonons by calculating the electron-phonon coupling in two different facets. Although in a slab phonon band, the [100] plane shows obvious surface phonon states, the electron-phonon coupling is surprisingly reduced, as compared to the [001] phase. Through this, we realize a competing relation between the electron-phonon coupling and the surface phonon bands. The former requires high symmetric stable bonding while the latter favors surface with dangling bond vibrations. A new mechanism of topological phonons toward surface superconductivity is still in search.

５． Schedule and prospect for the future

The future prospect of this project is to not go for the facet dependent of the topological phonons, which is also called the Zak phase mechanism. Next, by carefully examining the stable facet available for experiments, we could find other Weyl of Dirac phonons and calculate the electron-phonon coupling in the stable phonon facet.